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Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

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Abstract. Recently, an interface between the Monte Carlo code MCNPX and the neutron ray-tracing code MCNPX was developed [1, 2]. Based on the expected neutronic performance and guide geometries relevant for the ESS, the combined MCNPX-McStas code is used to calculate dose rates along neutron beam guides. The generation and moderation of neutrons is simulated using a full scale MCNPX model of the ESS target monolith. Upon entering the neutron beam extraction region, the individual neutron states are handed to McStas via the MCNPX-McStas interface. McStas transports the neutrons through the beam guide, and by using newly developed event logging capability, the neutron state parameters corresponding to un-reflected neutrons are recorded at each scattering. This information is handed back to MCNPX where it serves as neutron source input for a second MCNPX simulation. This simulation enables calculation of dose rates in the vicinity of the guide. In addition the logging mechanism is employed to record the scatterings along the guides which is exploited to simulate the supermirror quality requirements (i.e. m-values) needed at different positions along the beam guide to transport neutrons in the same guide/source setup.

1. Introduction

The European Spallation Source (ESS), presently starting construction in Lund, Sweden, will be the most intense source of spallation neutrons ever built [3]. Protons from a 5 MW, 2.5 GeV linear accelerator will impact a rotating tungsten target in 14, 2.86 ms long pulses every second. The spallation neutrons hereby created are thermalized in water and some of them are further cooled in liquid para-hydrogen before extracted through individual beam-lines serving 22 neutron scattering instruments¹. To fully exploit the long pulse characteristics, many instruments benefit from being long - up to 200 m is foreseen. Each instrument will be situated at the end of a guide tailored specifically to its requirements in terms neutron beam parameters. The design of the

¹ 22 is the foreseen number of instruments in the baseline facility design. Additional instruments may be added at a later stage.



guides is challenging and important since guides and in particular their shielding are a major cost driver for the ESS facility.

For these reasons it would be useful to have a tool that:

- Can monitor where in a guide neutrons are lost
- Allows to optimise reflectivity requirements along a guide
- Serves as an input for dose-rate calculations along the guide (n, γ)
- Works within the work-flow accustomed to instrument designers (McStas)

The newly developed tool *McStas Scatterlogger* is the backbone that facilitates this usage. Note that the examples of usage outlined below, to some limited extent are inspired by guide work relevant for the ESS, but the tool is general and can be used to assess neutron scatterings at any neutron scattering instrument.

2. McStas Scatterlogger: Implementation and usage

McStas [4, 5, 6] combines ray-tracing with Monte Carlo methods to accurately and efficiently simulate neutron scattering experiments of all types. As seen from the user perspective (typically instrument designers and users) the program is based upon a so-called *instrument file* in which you place predefined or user-supplied *components* according to the real setup of the instrument in question. The *instrument file* is written in a simple meta language, which at runtime is compiled first to the ansi-C programming language, which in turn is translated to an executable.

The *Scatterlogger* is an additional McStas component which can be placed in an *instrument file* wrapping around any other component - for example a guide component. At each scattering in the guide, the incoming and outgoing neutron state is then temporarily stored, and an iterator is supplied so that the user can analyse the scatterings once the neutron has exited the component. To prevent memory built-up the results of the analysis are stored in histograms, memory is flushed and McStas proceeds to the next neutron - as in any other McStas simulation.

In the intermediate analysis step (event post-processing), the user has access to the full neutron state before the scattering as well as the reflected and transmitted neutron state:

$$\begin{aligned}
 \text{Incoming state : } n_{in} &= (\mathbf{x}, \mathbf{v}_{in}, \mathbf{t}, \mathbf{w}_{in}) \\
 \text{Transmitted state : } n_{trans} &= (\mathbf{x}, \mathbf{v}_{in}, \mathbf{t}, \mathbf{w}_{trans}) \\
 \text{Reflected state : } n_{refl} &= (\mathbf{x}, \mathbf{v}_{out}, \mathbf{t}, \mathbf{w}_{in} - \mathbf{w}_{trans})
 \end{aligned} \tag{1}$$

Figure 1 contains a visualisation of a guide and the logging utility in operation. At each scattering of the neutron on the guide wall, the un-reflected neutron weight fraction is emitted as a secondary ray, propagated to a monitor component. The reflected neutron proceeds rightwards, traversing the guide with reduced weight.

3. Use-case 1: Lost intensity

This simple example considers a straight guide described by the parameters outlined in table 1 - see figure 1 for a visualization. At each scattering the transmitted weight w_{trans} and the corresponding position along the guide, z , is stored in a histogram and the result is shown in figure 2.

As expected the neutron loss occurs predominately at the first scattering in the beginning of the guide - the strength of the scatterlogging procedure is that it provides a method to quantify this. Obviously the extent at which intensity is lost along a guide depends strongly on the guide geometry and coating as well as the source (ie. energy, divergence and spatial extent). Thus, the

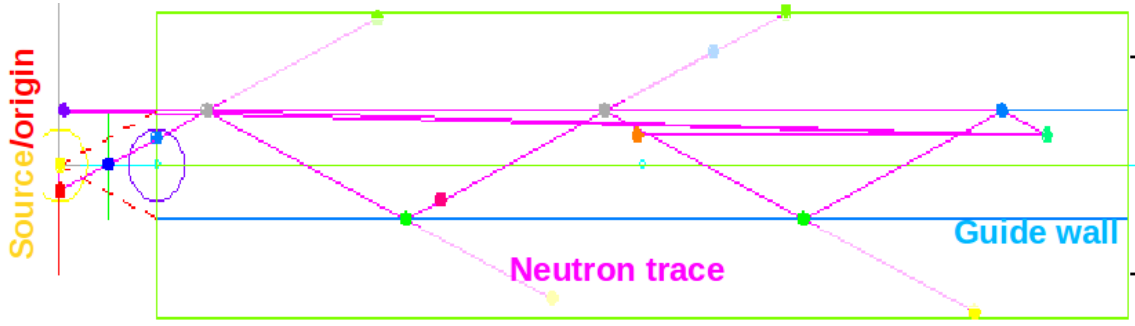


Figure 1. Basic guide geometry - from McStas' *mcdisplay*. Also shown in the figure is an example neutron trajectory. At each encounter with the guide wall, both the reflected and un-reflected neutron ray is stored and both trajectories are visualised. The un-reflected ray is allowed to propagate to a monitor component (green) surrounding the guide where it is detected. The apparent reflection (backscattering) from the right-most scattering back to the origin, is an (unphysical) feature of the visualization procedure.

Parameter	Value
guide length	10 m
guide coating	$m = 2$
cross-section of guide	10 cm \times 10 cm
source radius	10 cm
source spectrum	flat in wavelength: [0-10] Å
distance from source to guide entrance	1 m

Table 1. Parameters for the guide and source used in Use-cases 1 and 2. The source is focussed to illuminate precisely the guide entrance and nothing more.

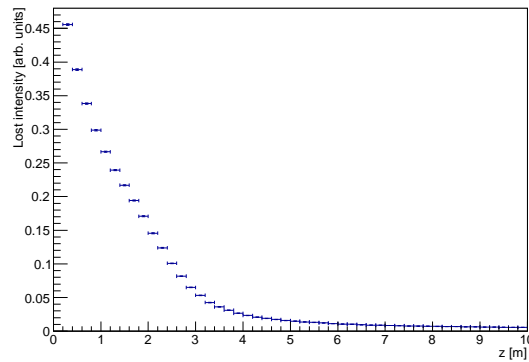


Figure 2. Histogram showing the lost neutron intensity along the straight guide as described in the text.

present example is by no means an attempt to describe guide losses in general, on the contrary the scatterlogging must be utilised individually to aid a particular guide design. Moreover, users should anticipate an iterative process where the results of one iteration (eg. figure 2) gives input to next - eg. increasing the m_{value} in the part of the guide closest to the source.

4. Use-case 2: Reflectivity

Neutrons scattering on a mirror are reflected if the energy/incident angle is sufficiently low. Specifically, the following relations hold (see figure 3):

$$\cos(2\theta) = (\vec{v}_{in} \cdot \vec{v}_{out}) / |\vec{v}_{in}|^2 \quad (2)$$

$$k = |\vec{v}_{in}| m_h / \hbar \quad (3)$$

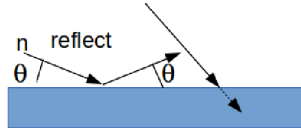


Figure 3. Reflected vs. absorbed neutron.

Given a neutron state and a guide geometry, the minimum mirror reflectivity requirement which would reflect the neutron, m_{min} , can be calculated [6]²:

$$m_{min} = 2 \cdot k \cdot \sin(\theta) / 0.0219 \text{ \AA}^{-1} \quad (4)$$

Figure 4 shows m_{min} for the first, second and third reflection respectively. The fact that the mirror in this example has an m_{value} of 2, is seen (on the intensity scale on the right-hand side of each figure) to cause significant loss of neutrons, in particular when comparing the first and second reflection.

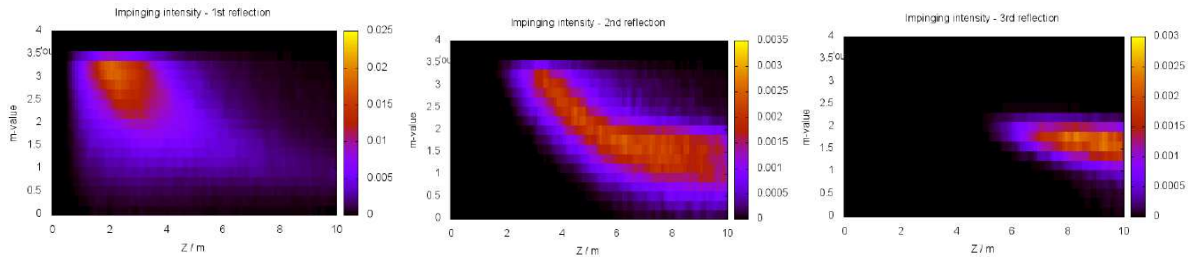


Figure 4. Histograms showing the minimum m -value required for a reflection, as a function of the position z along guide in a simulation of the 10 m straight guide described in the text. The color scale indicates the bin intensity. Note that the simulation was carried out using a $m = 2$ guide, which is seen to cause significant intensity loss in the beginning of the guide.

² Note that the value for Nickel reflectivity of 0.0219 is used for consistency with McStas default, despite that the standard value is 0.02175 \AA^{-1} .

5. Conclusions and outlook

The McStas Scatterlogger has proved a useful tool in guide design. In particular, it facilitates to monitor where along a guide neutron intensity is lost and allows to optimise where to use high-reflectivity mirror sections, and where less expensive mirrors can be installed with insignificant performance loss. Note that the results depend strongly on the simulated guide geometry and source specifications, wherefore simulations involving the McStas scatterlogger need to be performed based on individual guide\instrument designs.

The software needed to reproduce Use-cases 1 and 2 is available here: [7].

Future foreseen (or possible) extensions include the calculation of dose-rate along guides, backgrounds at the sample and detector position, activation calculations as well as calculation backgrounds and dose-rates at one instrument, caused by neutrons escaping a neighbouring instrument.

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